Positronium formation from Li and Na atoms by use of pseudopotentials

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The differential and total cross sections for the formation of positronium in its ground state from Li and Na atoms by the impact of intermediate-energy positrons are calculated in the first Born and distorted-wave Born approximations. Hellmann-type pseudopotentials are used to represent the alkali-metal ion cores. The difference in the use of pseudopotentials and the static potential for the core representation for evaluating various rearrangement cross sections is discussed.

I. INTRODUCTION

There has been a growing interest in the investigation of electron capture from alkali-metal atom. As an example, charge-transfer processes with Li have been suggested to be occurring in plasma diagnostic probes.[1] Also, alkali-metal atoms are many-electron systems that can be simplified to be one-electron systems due to a single valence electron. Theoretical calculations as well as experimental measurements have been carried out for ionization of and electron capture from alkali-metal atoms by proton impact (for some recent works see Refs. 1 and 2). The charge-transfer[3] and the total collisional[4] cross sections for positron impact on alkali-metal atoms have been calculated by several authors, and the total collisional cross sections have been measured for a potassium target by Stein *et al.*[5] In the present paper, the first Born approximation (FBA) and the distorted-wave Born approximation (DWBA) are used to calculate the cross sections for the ground-state positronium (Ps) formation from lithium and sodium by the impact of intermediate-energy positrons. Although the FBA cross sections are calculated and compared both in the post and the prior forms, DWBA cross sections are calculated, for computational convenience, only in the post form.

To compare the effects of different potentials (model potential versus pseudopotential) describing the ion cores, the first calculation[6] is done to calculate the cross sections for positronium formation from Li in the first Born approximation by using the static potential for the lithium ion core. The next calculations, employing FBA and DWBA, are for the positronium formation in both lithium and sodium using the pseudopotentials. In these calculations the alkali-metal ion cores have been represented by Hellmann-type pseudopotentials. A significant difference, in the values as well as in the shape, is observed for differential cross sections (DCS) in FBA using the pseudopotential and the static potential. A discussion about the formulation of various potentials representing the ion cores and the resulting differences in the shape of the DCS is presented in Secs. II B and III.

II. THEORY

A. Rearrangement cross sections

Let a positron of mass M_p with lab impact energy E and velocity $\mathbf{v}$ collide with a target alkali-metal atom at rest and form positronium in the ground state by electron capture from the target (T). Because of the single valence electron it is reasonable to treat the alkali-metal atom as a hydrogenic system by representing the ion core by a central potential, $V_p(r)$, which could either be a pseudopotential or a model potential. Then the initial and the final channel interactions are

$$V_i(\mathbf{r}_p,\mathbf{R}) = V_{p\text{-}e}(\mathbf{r}_p) + V_{p\text{-}T}(\mathbf{R}) = -e^2/r_p + V_p(R)\ , \tag{1a}$$

$$V_f(\mathbf{r}_T,\mathbf{R}) = V_{T\text{-}e}(\mathbf{r}_T) + V_{p\text{-}T}(\mathbf{R}) = V_p(r_T) + V_p(R)\ , \tag{1b}$$

respectively. The position vectors are shown in Fig. 1. The notation used is similar to that of Ref. 7. The interaction between the projectile and the valence electron is represented by $V_{p\text{-}e}$, that between the projectile and the target ion core is represented by $V_{p\text{-}T}$, and that between the target ion core and the electron is represented by $V_{T\text{-}e}$. In the present work $V_p(r)$ is chosen to be of the Hellmann or Yukawa type:[8]

$$V_p(r) = -\frac{e^2}{r} + \frac{e^2 A}{r}\exp(-\zeta r) - \frac{e^2\alpha_d}{2(r^2+d^2)^2} - \frac{e^2\alpha_q}{2(r^2+d^2)^3}\ . \tag{2}$$

The parameters A and ζ for the valence electron in lithium and sodium atoms are listed in Ref. 8. α_d and α_q are the dipole and the quadrupole polarizability, respectively, of the alkali-metal ion core. Both the valence electron and the projectile positron experience the same interaction with the atomic core except that the signs of the first two terms of V_p change in the case of the positron interaction.

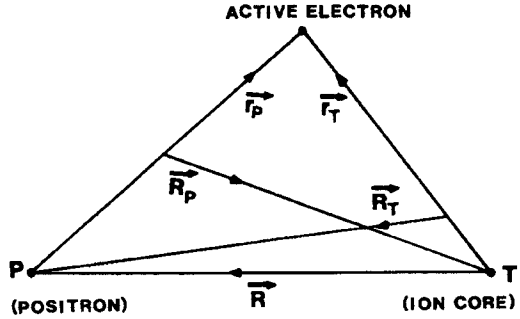

FIG. 1. Coordinate system.

This assumption is believed to be plausible for the following reasons. In the case of alkali-metal atoms the single valence electron is far removed from the alkali-metal ion core which contains the other tightly bound electrons and, therefore, the exchange effects in the valence-electron—ion-core interaction are expected to be small. Furthermore, the exchange interaction is, in general, a short-range and much weaker interaction compared to the static interaction. There are, of course, no exchange effects in positron—ion-core interactions. Thus, it appears reasonable to assume that in the energy range being considered here the valence electron and the incident positron experience similar interactions, apart from the sign of some terms, with the alkali-metal ion core. Defining the quantities

$$\alpha \equiv M_T/(m+M_T), \quad \beta \equiv M_p/(m+M_p) , \tag{3}$$

where m is the electron mass and M_T is the mass of the alkali-metal ion core, the various position vectors of Fig. 1 are related as

$$\begin{aligned} \mathbf{R}_T &= \mathbf{R}_p - (1-\beta)\mathbf{r}_p , \\ \mathbf{r}_T &= \mathbf{R}_p + \beta \mathbf{r}_p , \\ \mathbf{R} &= \mathbf{R}_T + (1-\alpha)\mathbf{r}_T , \\ \mathbf{R}_p &= \beta \mathbf{R}_T + (1-\alpha\beta)\mathbf{r}_T , \\ \mathbf{r}_p &= -\mathbf{R}_T + \alpha \mathbf{r}_T . \end{aligned} \tag{4}$$

$\mathbf{R}_T$ is the position vector of the positron relative to the center of mass of the alkali-metal atom and $\mathbf{R}_p$ is that of the ion core relative to the center of mass of the final bound state, Ps. The reduced masses are

$$\begin{aligned} \mu_T &= mM_T/(m+M_T) = \alpha m , \\ \mu_p &= mM_p/(m+M_p) = \beta m , \\ \nu_i &= M_p(m+M_T)/(m+M_T+M_p) , \\ \nu_f &= M_T(m+M_p)/(m+M_T+M_p) . \end{aligned} \tag{5}$$

In the center-of-mass frame, the total energy of the system is

$$E = \hbar^2 k_i^2/(2\nu_i) + \varepsilon_i = \hbar^2 k_f^2/(2\nu_f) + \varepsilon_f , \tag{6}$$

where $\hbar \mathbf{k}_i = \nu_i \mathbf{v}$ is the initial relative momentum and $\hbar \mathbf{k}_f$ is the final relative momentum, ε_i is the internal energy of the $(e+T)$ system, and ε_f is the internal energy of the final bound Ps state. The average momentum transfer vectors are

$$\mathbf{K} = \beta \mathbf{k}_f - \mathbf{k}_i, \quad \mathbf{J} = \alpha \mathbf{k}_i - \mathbf{k}_f . \tag{7}$$

If Ψ_i^+ is the exact wave function of the complete system in the initial channel with outgoing wave boundary conditions, then the Schrödinger equation satisfied by Ψ_i^+ is

$$\left[-\frac{\hbar^2}{2\nu_i}\nabla_{\mathbf{R}_T}^2 - \frac{\hbar^2}{2\mu_T}\nabla_{\mathbf{r}_T}^2 + V_i + V_{Te} \right] \Psi_i^+ = E\Psi_i^+ , \tag{8}$$

which, for the purpose of using the two-potential theory, can be rewritten as

$$[H_D + (V_i - U_i)]\Psi_i^+ = E\Psi_i^+ , \tag{9}$$

where

$$H_D = H_0 + U_i + V_{Te}, \quad H_0 = -\frac{\hbar^2}{2\nu_i}\nabla_{\mathbf{R}_T}^2 - \frac{\hbar^2}{2\mu_T}\nabla_{\mathbf{r}_T}^2 , \tag{10}$$

and U_i is as yet an arbitrary distortion potential. The distorted wave χ_i^+, then, is

$$\chi_i^+ = \psi_i^+ \frac{1}{E - H_D + i\varepsilon} U_i \psi_i , \tag{11}$$

where χ_i^+ and ψ_i satisfy

$$H_D \chi_i^+ = E\chi_i^+ \text{ and } (H_0 + V_{Te})\psi_i = E\psi_i . \tag{12}$$

Similar forms for the different wave functions $(\Psi_f^-, \chi_f^-, \psi_f$, etc.) can be obtained for the final channel. Let $\phi_i(\mathbf{r}_T)$ represent the internal state of $(e+T)$ such that

$$\left[-\frac{\hbar^2}{2\mu_T}\nabla_{\mathbf{r}_T}^2 + V_{Te} \right] \phi_i(\mathbf{r}_T) = \varepsilon_i \phi_i(\mathbf{r}_T) . \tag{13}$$

A similar equation could be written for the final internal state $\phi_f(\mathbf{r}_p)$ of Ps. The initial and final channel wave functions are then

$$\psi_i = \exp(i\mathbf{k}_i \cdot \mathbf{R}_T)\phi_i(\mathbf{r}_T), \quad \psi_f = \exp(i\mathbf{k}_f \cdot \mathbf{R}_p)\phi_f(\mathbf{r}_p) , \tag{14}$$

respectively. If χ_i^+ is chosen, following Ref. 7, to be of the form

$$\chi_i^+ = \phi_i(\mathbf{r}_T)[\exp(i\mathbf{k}_i \cdot \mathbf{R}_T) + g_i^+(\mathbf{R}_T)] , \tag{15}$$

then it follows from Eq. (11) that

$$g_i^+ \phi_i(\mathbf{r}_T) = \frac{1}{E - H_D + i\varepsilon} U_i \psi_i . \tag{16}$$

Upon operating on both sides of Eq. (16) by $(H_D - E)$, using Eq. (13) and then taking the Fourier transform of the resulting equation, it is seen that $\tilde{g}_i^+$ satisfies

$$\tilde{g}_i^+(\mathbf{K})\hbar^2(K^2 - k_i^2 - i\eta)/(2\nu_i) + \tilde{U}_i(\mathbf{K} - \mathbf{k}_i) + (2\pi)^{-3/2} \int \tilde{g}_i^+(\mathbf{p})\tilde{U}_i(\mathbf{K} - \mathbf{p}) d^3p = 0 . \tag{17}$$

Here the tilde represents the Fourier transform. Similarly, for the final channel, if one writes

$$\chi_f^- = \phi_f(\mathbf{r}_p)[\exp(i\mathbf{k}_f \cdot \mathbf{R}_p) + g_f^-(\mathbf{R}_p)] , \tag{18}$$

then an integral equation, similar to Eq. (17), can be obtained for $\tilde{g}_f^-$. The integral equations can be solved to first order in the distortion potentials U_i and U_f to give

$$\tilde{g}_i^+(\mathbf{K}) = -\frac{2\nu_i}{\hbar^2} \frac{\tilde{U}_i(\mathbf{K} - \mathbf{k}_i)}{K^2 - k_i^2 - i\eta} , \tag{19}$$

and

$$\tilde{g}_f^-(\mathbf{K}) = -\frac{2\nu_f}{\hbar^2} \frac{\tilde{U}_f(\mathbf{K} - \mathbf{k}_f)}{K^2 - k_f^2 + i\eta} . \tag{20}$$

The specific forms chosen for the distortion potentials are the static potentials

$$\begin{aligned} U_i(\mathbf{R}_T) &= \int |\phi_i(\mathbf{r}_T)|^2 V_i(\mathbf{r}_p, \mathbf{R}) d^3 r_T , \\ U_f(\mathbf{R}_p) &= \int |\phi_f(\mathbf{r}_p)|^2 V_f(\mathbf{r}_T, \mathbf{R}) d^3 r_p . \end{aligned} \tag{21}$$

Since U_i depends only on $\mathbf{R}_T$ and U_f depends only on $\mathbf{R}_p$, the T-matrix element for the transition from the initial state to the final state is given by[9]

$$T=\langle\chi_f^-\mid V_f-U_f\mid\Psi_i^+\rangle\ , \tag{22a}$$

in the post form, and

$$T=\langle\Psi_f^-\mid V_i-U_i\mid\chi_i^+\rangle\ , \tag{22b}$$

in the prior form. If the perturbations (V_i-U_i) and (V_f-U_f) are weak enough, Ψ_i^+ and Ψ_f^- can be replaced by χ_i^+ and χ_f^-. This approximation is the distorted-wave Born approximation (DWBA) used here, and the T-matrix element in this approximation is given by

$$T=\langle\chi_f^-\mid V_f-U_f\mid\chi_i^+\rangle\ , \tag{23a}$$

in the post form, and

$$T=\langle\chi_f^-\mid V_i-U_i\mid\chi_i^+\rangle\ , \tag{23b}$$

in the prior form. The present DWBA calculations for the positronium formation from alkali-metal atoms have been done in the post form only. The T-matrix element in the post form is

$$T=T_1+T_2+T_3\ , \tag{24}$$

where

$$\begin{aligned}T_1&=\langle\psi_f\mid V_f-U_f\mid\psi_i\rangle\ ,\\ T_2&=\langle\psi_f\mid V_f-U_f\mid g_i^+\phi_i\rangle\\ &\quad+\langle g_f^-\phi_f\mid V_f-U_f\mid\psi_i\rangle\equiv T_2^+ +T_2^-\ ,\\ T_3&=\langle g_f^-\phi_f\mid V_f-U_f\mid g_i^+\phi_i\rangle\ .\end{aligned} \tag{25}$$

Note, on using Eqs. (19) and (20), that T_1, T_2, and T_3 are first, second, and third order in the potential, respectively. Then keeping consistently terms up to third order in the potential, the differential cross section is

$$\left[\frac{d\sigma}{d\Omega}\right]_{\rm DWBA}=\frac{\nu_i\nu_f k_f}{4\pi^2\hbar^4 k_i}\mid T\mid^2\ , \tag{26}$$

where

$$\mid T\mid^2=\{\mid T_1\mid^2+2[{\rm Re}(T_1){\rm Re}(T_2)+{\rm Im}(T_1){\rm Im}(T_2)]\}\ . \tag{27}$$

When distortion is excluded, the first Born approximation is obtained for which

$$T=\langle\psi_f\mid V_f\mid\psi_i\rangle\ , \tag{28a}$$

in the post form, and

$$T=\langle\psi_f\mid V_i\mid\psi_i\rangle\ , \tag{28b}$$

in the prior form. The cross sections for positronium formation in FBA have been calculated both in the post and the prior forms in order to check the accuracy of the trial wave functions for the valence electron of the alkali-metal atom. A better trial wave function, obtained by a lowering of the energy in the variational principle, results in a smaller post-prior discrepancy. The integrated cross section for positronium formation

$$\sigma=2\pi\int_0^\pi\left[\frac{d\sigma}{d\Omega}\right]\sin\theta\,d\theta \tag{29}$$

is evaluated numerically.

Atomic units are used in the present calculations. In these calculations the pseudopotential, Eq. (2), has been reduced without losing much accuracy to

$$V_p(r)=-1/r+(A/r)\exp(-\zeta r) \tag{30}$$

for computational ease. The parameters A and ζ for the valence electron in lithium and sodium atoms are taken from Ref. 8. It was found that even without the polarization terms for the ion cores in $V_p(r)$ the use of Eq. (30) in Eq. (13) gives the energy ε_i of the valence electron in the alkali-metal atom very close to the observed values. The value of ε_i obtained in the present calculations is $-0.195\,895\,6$ a.u. compared to $-0.198\,162\,4$ a.u.[10] for the $2s$ valence electron of Li and $-0.182\,596$ a.u. compared to $-0.188\,864\,4$ a.u.[10] for the $3s$ valence electron of Na. The trial wave function for the s-state valence electron is expanded in terms of hydrogenic wave functions as

$$\phi_i(\mathbf{r})=Y_{00}(\hat{\mathbf{r}})\sum_{m=1}^{3}\sum_{l=1}^{2}c_{l+2m-2}r^{l-1}\exp(-\delta_m r)\ , \tag{31}$$

where c_l and δ_m are variational parameters. Writing the distortion potential as

$$U_i(\mathbf{R}_T)=\int\mid\phi_i(\mathbf{r}_T)\mid^2 V_{pe}(\mathbf{r}_p)d^3r_T+V_p(R_T)\ , \tag{32}$$

where it is assumed that $\alpha=1$ in the second term, the Fourier transform of the distortion potential can be written as

$$\tilde{U}_i(\mathbf{K})=\frac{1}{\sqrt{2\pi}}\left[-\frac{A}{\zeta^2+K^2}+\sum_{m=1}^{3}\sum_{n=1}^{3}\sum_{l=0}^{3}(-1)^l Q_{mnl}\frac{d^l}{dx^l}\frac{1}{x^2+K^2}\right]\ ,$$

where

$$\begin{aligned}Q_{mn0}&=c_{2m-1}c_{2n-1}D_2+(c_{2m-1}c_{2n}+c_{2n-1}c_{2m})D_3+c_{2m}c_{2n}D_4\ ,\\ Q_{mn1}&=c_{2m-1}c_{2n-1}D_1+2(c_{2m-1}c_{2n}+c_{2n-1}c_{2m})D_2+3c_{2m}c_{2n}D_3\ ,\\ Q_{mn2}&=(c_{2m-1}c_{2n}+c_{2m}c_{2n-1})D_1+3c_{2m}c_{2n}D_2\ ,\quad Q_{mn3}=c_{2m}c_{2n}D_1\ ,\quad x=\delta_m+\delta_n\ ,\quad D_i=i!/x^{i+1}\ .\end{aligned} \tag{33}$$

The distortion potential in the final channel is

$$U_f(\mathbf{R}_p)=\int |\phi_f(\mathbf{r}_p)|^2[V_p(R)+V_p(r_T)]d^3r_p \ . \quad (34)$$

It vanishes when $\beta=\frac{1}{2}$ as in the case of Ps formation. Hence g_f^- also vanishes. The terms involved in calculating the cross sections in the post and prior forms of FBA and in the post form of the DWBA are given in the Appendix.

B. Pseudopotentials for rearrangement processes

Consider an N-electron open-shell atom with Z valence electrons. The general distinction between the valence and the core electrons is that the valence electrons determine many of the physical and chemical properties of the atom while the core electrons are relatively inert. Therefore, in a moderate-energy collision process it is a fairly good approximation to assume that the valence (or the outer electrons) take part in the interactions while the core electrons remain essentially inactive. However, for calculational purposes one needs to know the wave functions of the valence as well as the core electrons, that is, the total wave function of the atom which is antisymmetric with respect to the interchange of any pair of electrons. In the Hartree-Fock approximation this wave function is an $N\times N$ determinant of one-electron wave functions which are orthogonal to each other. In order to avoid the complications associated with the orthogonalization of N one-electron wave functions, one can utilize either a model or a pseudopotential approach. In the pseudopotential procedure the problem of N electrons is simplified by reducing it to a problem of Z electrons by introducing a repulsive potential $V(\mathbf{r})$ along with the ordinary Coulomb and exchange potentials for the valence electrons. This repulsive part represents the partially screened nucleus and simulates the orthogonality condition or Pauli principle by keeping the valence electrons out of the core. It may also contain implicitly the correlation between the valence and the core electrons which is generally expressed by the polarization potential. In its general form the radial part of $V(\mathbf{r})$ can be a Hellmann (or Yukawa) type, a Gaussian type, or a combination of various short-range potential terms. The difference between this choice of the potential for the core and the Hartree-Fock potential is that in the former case there are no energy eigenvalues corresponding to the core electrons, and the valence-electron wave functions are nodeless for s electrons, have one node for p electrons, etc. Hence the lowest Z eigenvalues correspond to the energies of the Z valence electrons.

The concept of the pseudopotential in atomic, molecular, nuclear, and condensed-matter physics has been known for quite a long time. Since the independent introductions of the pseudopotential, semiempirically by Hellmann,[11] and on the basis of the statistical model of the atom by Gombas,[12] the method of pseudopotential formulations has been developed by many investigators,[13] and several review articles[14] on this subject have been written. We will concentrate on determining the pseudopotential parameters for atoms with a single valence electron—for example, the alkali-metal atoms. Following the pseudopotential method as suggested by Hellmann, the Schrödinger equation for the valence electron (in a.u.) is

$$[-\tfrac{1}{2}\nabla^2+V_p(r)]\phi(\mathbf{r})=\varepsilon\phi(\mathbf{r}) \ ,$$

where

$$V_p(r)=-1/r+(A/r)\exp(-\zeta r) \quad (35)$$

is the effective potential for the valence electron. A and ζ are variational parameters, ε is the binding energy of the valence electron, and $\phi(\mathbf{r})$ is the wave function of the valence electron, not necessarily orthogonal to the wave functions of the core electrons. Generally, $\phi(\mathbf{r})$ is approximated by a trial wave function of the form

$$\phi(\mathbf{r})\sim\sum_{m,n,l} R_{nl}(r)Y_{lm}(\hat{\mathbf{r}}) \ , \quad (36)$$

where the radial part $R_{nl}(r)$ contains one or a few terms (depending on the atomic state it is representing) of hydrogenic functions with some adjustable parameters. The parameters A and ζ of the pseudopotential and the adjustable parameters of the wave function R_{nl} are varied until the lowest few eigenvalues, obtained using the Ritz variational principle, agree as well as possible with the observed energies of the ground and the first few excited states. This procedure for determining the potential can fail since on increasing the number of terms in the expansion for $R_{nl}(r)$, the energy eigenvalues ε of Eq. (35) continue to decrease and eventually can become much lower than the experimental values.

The alternate way to determine the values of the pseudopotential parameters is to solve Eq. (35) by direct numerical integration using the Numerov method. The radial part of the bound state $\phi(\mathbf{r})$ behaves as

$$\begin{aligned} &R_{nl}(r)\sim r^l \ \text{ for } r\to 0 \ , \\ &R_{nl}(r)\sim\exp(-\sqrt{F}r)/r \ \text{ for } r\to\infty \ , \end{aligned} \quad (37)$$

where $F=2(V_p-\varepsilon)$. Using the conditions of Eq. (37), the outward and the inward radial wave functions are generated and matched at a suitable matching radius. The first Kato cusp condition[15] can be used to start the outward function near the origin. The parameters A and ζ are varied until both the wave function and its derivative become continuous at the matching point. For a fixed energy ε of the valence electron a number of sets of parameter values may be obtained which will generate a smooth wave function for the ground state. Only that set of parameters is to be chosen which will reproduce as closely as possible a few low-lying energy levels of the same symmetry. In Ref. 8, from which the present values of A and ζ for the valence electron in Li and Na are taken, the parameters were chosen so that the lowest two energy levels were reproduced exactly. It is to be noted that a wave function which closely reproduces an energy eigenvalue may not necessarily generate expectation values of various powers of r which would agree with the previously known values[16] of these matrix elements. It is then possible that the transition matrix elements relevant to collisional processes could be affected which, in turn, would affect the related cross sections.

To illustrate the use of different potentials, the cross sections for positronium formation from Li by the impact of positrons have been calculated[6] using the static potential of the Li^+ core in the FBA. The static potential experienced by the valence electron is obtained by averaging the instantaneous interaction over the motion of the core electrons:

$$V_s(r)=\int |\Phi(\mathbf{r}_1,\mathbf{r}_2)|^2 \times\left[-\frac{1}{r}+\frac{1}{|\mathbf{r}-\mathbf{r}_1|}+\frac{1}{|\mathbf{r}-\mathbf{r}_2|}\right]d\mathbf{r}_1 d\mathbf{r}_2 . \quad (38)$$

$\Phi(\mathbf{r}_1,\mathbf{r}_2)$ is the antisymmetric Hartree-Fock wave function of Li^+ in terms of one-electron Slater-type orbitals given by Clementi and Roetti.[17] Since it is determined by the exact interaction and the Hartree-Fock functions, the static potential can be considered a model potential and not a pseudopotential. Unlike a pseudopotential, a model potential has bound states which may not correspond in energy to the observable states of the atom. Hence the lowest energy eigenvalue of the model Hamiltonian may not necessarily correspond to the energy of the valence electron. However, the wave function of the valence electron has the correct number of nodes, namely, $n-l-1$. The difference between the pseudopotential and the model-potential approaches has been discussed and elaborated on by Peach.[18] A six-term trial wave function for the $2s$ valence electron of the Li atom, similar to Eq. (31), which corresponds to an energy value of $-0.175\,867$ a.u. for the valence electron (that is, the second lowest eigenvalue of the Hamiltonian) in the static potential $V_s(r)$ of Li^+, is used for the calculations of the cross sections for positronium formation in FBA. The differential cross sections are shown in Fig. 2, and the integrated cross sections are given in Table I.

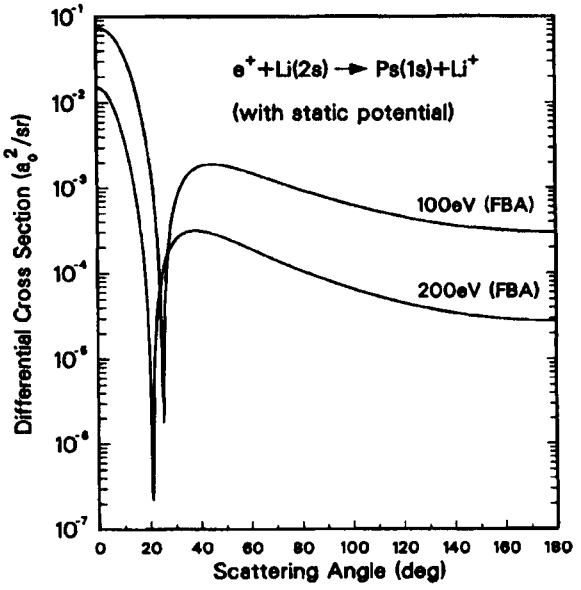

FIG. 2. Differential cross sections for the positronium formation from Li at positron impact energies of 100 and 200 eV using FBA.

III. RESULTS AND DISCUSSION

The differential cross sections (DCS), using the FBA, for the formation of positronium at positron impact energies of 100 and 200 eV from Li are shown in Fig. 2, and the integrated cross sections are presented in Table I. In these calculations, a static potential has been used to represent the alkali-metal ion core. The DCS and the integrated cross sections using both the FBA and the DWBA for the formation of positronium from Li and Na using pseudopotentials for the representation of the alkali-metal ion cores are also calculated. These DCS values for a Li target at positron impact energies of 100 and 300 eV are shown in Fig. 3, and for a Na target at positron impact energies of 75, 200, and 300 eV are shown in Fig. 4. The corresponding integrated cross sections are provided in Table I. In order to obtain the energy values and the wave function parameters for the valence electron of the alkali-metal atoms in Eq. (13), the variational principle as well as direct numerical integration using the Numerov method is used. The post-prior discrepancy for both the DCS and the integrated cross sections in the FBA is negligibly small in all cases. Hence only the post results in FBA are shown in Figs. 2–4. Some differences in the values of the cross sections, using the pseudopoten-

TABLE I. The integrated cross sections using FBA (σ_{FBA}) and DWBA (σ_{DWBA}) for Ps($1s$) formation from Li and Na by the impact of positrons. The notations p and s following the target atom correspond to the use of pseudopotential and static potential, respectively. Numerical values of the form $a[b]$ mean $a\times10^b$.

Target atom	Positron impact energy (eV)	σ_{FBA} (units of a_0^2) Post	Prior	σ_{DWBA} (units of a_0^2) Post
Li(p)	100	8.4317[−2]	8.430[−2]	2.8105[−1]
	300	1.8319[−3]	1.8334[−3]	2.254 65[−3]
Na(p)	75	3.5692	3.5676	1.3882[2]
	200	1.7259[−1]	1.7271[−1]	3.7385
	300	1.1783[−2]	1.1775[−2]	1.8342[−1]
Li(s)	50	6.3872[−2]	6.4361[−2]	
	100	1.9632[−2]	1.9704[−2]	
	200	2.5137[−3]	2.5023[−3]	

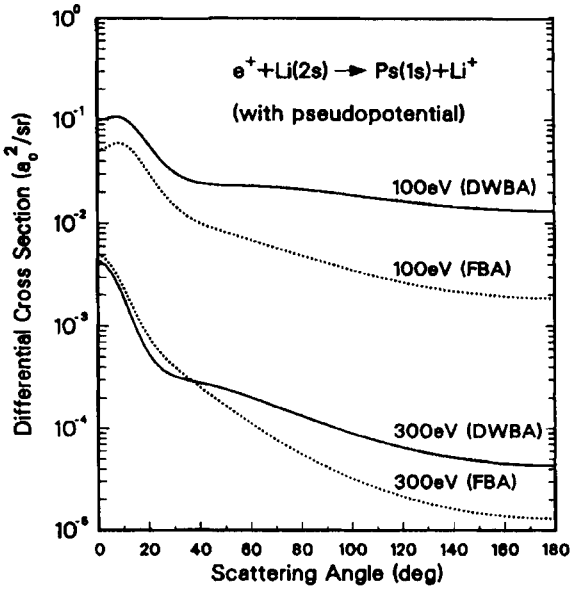

FIG. 3. Differential cross sections for the positronium formation from Li at positron energies of 100 and 300 eV using both the FBA and the DWBA.

tial and the static potential, are expected since the two potentials representing the Li^+ core do not correspond exactly to the same energy eigenvalue for the $2s$ valence electron. This difference is obvious in the values of Table I. Not only the values but also the shapes of the differential-cross-section curves, as shown in Figs. 2 and 3, are different. While with the static potential the DCS curves show a sharp minimum that moves toward the forward direction with increasing impact energy, with the pseudopotential these curves show a maximum, prominent at lower energies, near the forward direction. The total positron-atom interaction potential has both an attractive and a repulsive part. In the calculation employing the static potential, the contribution to the scattering amplitude arising from the repulsive part of the interaction almost equals that from the attractive part for a certain angle which results in a minimum in the DCS curve. This angle depends on the positron impact energy. This minimum in the DCS curve has also been obtained by Guha and Saha[3] (using FBA) and Mazumdar and Ghosh[3] (using FBA and the distorted-wave polarized orbital method). Guha and Saha have used a core model potential different from the one used here and their results (evaluated in the post form) for the positronium formation cross sections are much lower than the present results. Mazumdar and Ghosh[3] have used only the static potential for the Li^+ ion core. Their calculated positronium formation cross section at 50-eV impact energy, using FBA, is comparable with the present result but their cross section at 100-eV impact energy is lower than the present one.

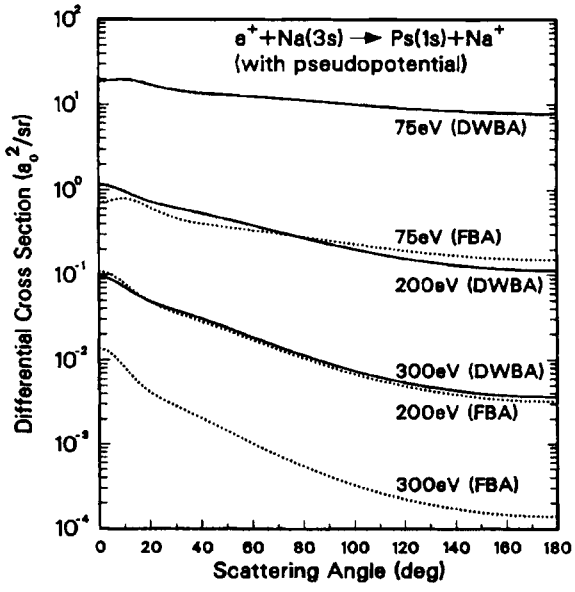

FIG. 4. Differential cross sections for the positronium formation from Na at positron impact energies of 75, 200, and 300 eV using both the FBA and the DWBA.

In the present calculations it is noticed that the contribution from the positron—ion-core interaction to the DCS values dominates at larger angles in all cases. Also in the present calculations, using the pseudopotential in DWBA, it is seen that the distortion contributes significantly to the positronium formation cross sections, especially for the Na target. No measured values for the corresponding cross sections with Li and Na targets are available at this moment, but such measurements may be feasible in the future.[19] Only when the experimental results become available in the future can a better justification for the use of different potentials be made. In spite of the availability of good wave functions containing the Slater-type orbitals[17] of alkali-metal atoms, the static potential formed by these wave functions does not provide the energy of the valence electron to a very good approximation. [See the energy values following Eqs. (30) and (38).] Furthermore, the form of these wave functions (having many terms) makes them computationally inconvenient for the evaluation of capture cross sections. In this respect the pseudopotentials are simpler to use, and the energy eigenvalues corresponding to these potentials can be made very close to the measured energy values of the alkali-metal atoms using adjustable parameters.

It is to be noted that, even though the model static potential and the pseudopotential do not reproduce the alkali-metal spectrum to the same degree of accuracy, a comparison between the positronium formation cross sections using these two potentials is still worthwhile. In the absence of any experimental information about cross sections for positronium formation in alkali-metal atoms, we can compare only with the previous theoretical results for these cross sections. The majority of these calculations[3] exhibited features in the positronium formation cross sections which were similar to the ones observed in Fig. 2 for the Ps formation in Li using the model static potential. We note that this potential did not reproduce the energies of the alkali-metal ground states very well. On the other

hand, use of the pseudopotential, which reproduces the energies of the alkali-metal ground states quite well, in the present calculations provides Ps formation cross sections which differ markedly in shapes and magnitudes from the previous calculations.

In the present calculations terms up to third order in the potential are kept in the cross-section expression with the assumption that the higher-order terms contribute less significantly. The cross-section integrals are simplified by the fact that the positron mass is much smaller than that of the alkali-metal ions ($\alpha=1$). Several checks were made to ensure the correctness of the present computer codes.

(a) Both the FBA and DWBA cross sections for the process $e^+ + H(1s) \rightarrow Ps(1s) + H^+$ at a positron impact energy of 100 eV (Ref. 7) were reproduced.

(b) The DCS values in FBA for the process $e^+ + H(1s) \rightarrow Ps(1s) + H^+$ at a positron impact energy of 500 eV (Ref. 20) were reproduced.

(c) The DCS values in FBA for the process $H^+ + H(1s) \rightarrow H(1s) + H^+$ at a proton impact energy of 700 keV (Ref. 20) were reproduced.

(d) The DCS values in FBA for the process $H^+ + H(1s) \rightarrow H(1s) + H^+$ at a proton impact energy of 198.344 keV (Ref. 21) were reproduced.

(e) An attempt to reproduce the DCS values in FBA for the process $e^+ + Li(2s) \rightarrow Ps(1s) + Li^+$, as reported by Guha and co-workers,[3] did not meet with success. A small computer program which specifically made use of the wave function and potential of Guha *et al.* was written. This program reproduced the same values of the differential cross section as given by our general program.

Finally, we comment on two aspects of the present calculations for positronium formation from alkali-metal atoms. First, the shapes of the differential cross sections for positronium formation depend on the type of interaction potential used in the calculations. This is obvious on comparing Figs. 2 and 3. It is not yet possible to ascertain the correctness of either shape due to the absence of corresponding experimental cross sections. The second remark concerns the significant difference in the values of the cross sections, both differential and integrated, obtained by using the FBA and the DWBA. A rather large difference between the two values seems to suggest that the higher-order distortion terms in the DWBA may contribute significantly to the cross sections. The importance of including these terms can only be determined when the experimentally measured values of the cross sections for positronium formation become available.

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APPENDIX

In this appendix we present analytical forms for various terms in the cross sections for positronium formation. Note that U_f vanishes for the positronium formation. Various parts of the post form T-matrix elements, Eq. (25), using DWBA can be written as

$$T_1 = N_1 + N_2 , \tag{A1}$$

where

$$N_1 = -(2\pi)^{3/2} \int \tilde{\phi}_f^*(\mathbf{K}-\mathbf{t}) \tilde{V}_p(\mathbf{t}) \tilde{\phi}_i(-\mathbf{t}-\mathbf{J}) d^3t , \tag{A2}$$

$$N_2 = (2\pi)^{3/2} \tilde{\phi}_f^*(\mathbf{K}) \int \tilde{V}_p(\mathbf{t}) \tilde{\phi}_i(-\mathbf{t}-\mathbf{J}) d^3t , \tag{A3}$$

$$T_2^+ = L_1 + L_2 , \tag{A4}$$

where

$$L_1 = -\int \tilde{\phi}_f^*(-\mathbf{t}-\mathbf{q}+\beta\mathbf{k}_f) \tilde{V}_p(\mathbf{t}) \tilde{g}_i^+(\mathbf{q}) \times \tilde{\phi}_i(-\mathbf{t}-\alpha\mathbf{q}+\mathbf{k}_f) d^3t\, d^3q , \tag{A5}$$

$$L_2 = \int \tilde{\phi}_f^*(-\mathbf{q}+\beta\mathbf{k}_f) \tilde{V}_p(\mathbf{t}) \tilde{g}_i^+(\mathbf{q}) \times \tilde{\phi}_i(-\mathbf{t}-\mathbf{q}+\mathbf{k}_f) d^3t\, d^3q . \tag{A6}$$

In evaluating L_1, is it assumed that $\alpha=1$. T_2^- and T_3 vanish because of the vanishing of g_f^-. In the prior form of FBA, the T-matrix element (Eq. 28) is given by

$$T = N_1 + N_3 , \tag{A7}$$

where N_1 is same as in Eq. (A2) and

$$N_3 = -(2\pi)^{3/2} [K^2/(2\mu_p) - \varepsilon_f] \tilde{\phi}_f^*(\mathbf{K}) \tilde{\phi}_i(-\mathbf{J}) . \tag{A8}$$

In the post form of FBA, the T-matrix element of Eq. (28) is essentially T_1 of Eq. (A1). The integrals involved in evaluating these terms are of the form

$$I_1 = \int d^3p \frac{1}{(\mathbf{p}-\mathbf{A})^2+a^2} \frac{1}{(\mathbf{p}-\mathbf{B})^2+b^2} \frac{1}{p^2+z^2} , \tag{A9}$$

$$I_{1p} = \int d^3p \frac{1}{[(\mathbf{p}+\mathbf{A})^2+a^2]^2} \frac{1}{p^2+z^2} , \tag{A10}$$

$$I_2 = \int\int d^3p\, d^3q \frac{1}{(\mathbf{p}-\mathbf{A})^2+a^2} \frac{1}{(\mathbf{p}-\mathbf{B})^2+b^2} \frac{1}{p^2-v^2-i\eta} \frac{1}{[(\mathbf{p}+\mathbf{q}-\mathbf{D})^2+d^2]^2} \frac{1}{q^2+z^2} , \tag{A11}$$

$$I_3 = \int\int d^3p\, d^3q \frac{1}{(\mathbf{p}+\mathbf{q}-\mathbf{A})^2+a^2} \frac{1}{(\mathbf{p}+\mathbf{q}-\mathbf{B})^2+b^2} \frac{1}{p^2+c^2} \frac{1}{(\mathbf{q}-\mathbf{D})^2+d^2} \frac{1}{q^2-v^2-i\eta} . \tag{A12}$$

I_{1p} is integrated analytically and is given by

$$I_{1p} = \frac{\pi^2}{a} \frac{1}{A^2+(a+z)^2} . \tag{A13}$$

Using a Feynman identity, as in Ref. 7, the other integrals are reduced as follows:

$$I_1 = \pi^2 \int_0^1 dx \frac{1}{E[F^2+(E+z)^2]} ,$$

where

$$E^2=x(1-x)(\mathbf{A}-\mathbf{B})^2+xa^2+(1-x)b^2\ ,$$
$$\mathbf{F}=(\mathbf{A}-\mathbf{B})x+\mathbf{B}\ , \tag{A14}$$
$$I_2=\frac{\pi^4}{d}\int_0^1 dx\int_0^1 dy\, y\left[\frac{1}{2s^3T}+\frac{s-iv}{s^2T^2}\right]\ ,$$

where

$$E^2=x(1-x)(\mathbf{A}-\mathbf{D})^2+xa^2+(1-x)(d+z)^2\ ,$$
$$\mathbf{F}=(\mathbf{A}-\mathbf{D})x+\mathbf{D}\ ,$$
$$s^2=y(1-y)(\mathbf{F}-\mathbf{B})^2+yE^2+(1-y)b^2\ , \tag{A15}$$
$$T=-v^2-2ivs+y(E^2+F^2)+(1-y)(b^2+B^2)\ ,$$
$$I_3=\pi\int_0^1 dx\int_0^1 dy\frac{1}{Es[T^2+(s-iv)^2]}\ ,$$

where

$$E^2=x(1-x)(\mathbf{A}-\mathbf{B})^2+xa^2+(1-x)b^2\ ,$$
$$\mathbf{F}=x(\mathbf{A}-\mathbf{B})+\mathbf{B}\ ,$$
$$s^2=y(1-y)(\mathbf{F}-\mathbf{D})^2+y(E+c)^2+(1-y)d^2\ , \tag{A16}$$
$$\mathbf{T}=y\mathbf{F}+(1-y)\mathbf{D}\ .$$

Now the integrals are evaluated numerically. The one-dimensional integrals have been integrated using Simpson's rule, and the two-dimensional integrals are evaluated using a 9-point square formula[22] with an error proportional to the sixth power of the stepsize.

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